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Solvation Science: A New Interdisciplinary Field

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The ancient philosopher Thales of Miletus (624–548 BC) conferred water a place of honor in his "Weltanschauung" (perception of the world) and an active role in the transformation of substances. Later on, the alchemists' frantic search for the "alkahest", a universal solvent capable of dissolving any substance, demonstrates the importance that solvation already had in the middle ages.

As we now know, the majority of chemical reactions and virtually all biological processes take place in a liquid-state environment, but there is no such thing as the alkahest. Solvents, with water being the most prominent, dissolve or "solvate" reagents and thereby transfer them as "solutes" into the liquid state; they also wet extended surfaces such as lipid membranes or metal electrodes, thus creating new interfaces. Solvation as a topic is thus at the very heart of chemistry as well as chemical engineering, but the original philosophical idea of solvents being active players has remained elusive for a long time.

By the end of the 19th century, scrupulous research on solvents performed by a group of collaborative chemists proved successful enough to provide the first theoretical laws governing solvation. Van't Hoff and Arrhenius were awarded the first (1901) and third (1903) Nobel Prizes in Chemistry for their work on the osmotic pressure of dilute solutions, and the ionization of substances in aqueous solutions, respectively. Together with other scientists such as Ostwald and Debye, they paved the way to a macroscopic, descriptive, and empirical view of solvents, which allowed chemists, physicists, engineers, and biologists developing their own viewpoints, models, and practical approaches to find the most efficient solvents. Solvents are often considered to be an inert media, in which reactions occur.

However, a top-down perspective on solvation processes developed on the basis of experimental trial and error has drawbacks: Continuing to apply such a strategy may well result in overlooking the best solutions to the scientific challenges ahead. Indeed, knowing that one solvent is more efficient than another for a certain chemical process doesn't tell us why this happens at a molecular level, nor if a third solvent might have better characteristics and, hence, confer greater efficiency. Finding the right solvents is a precondition for optimizing industrial processes, avoiding environmental hazards, preventing corrosion, or increasing energy efficiency, to name but a few challenges of our modern society. As George Whitesides recently pointed out in *Angewandte Chemie* in an Essay about the future of chemistry, understanding the role of water in the myriad of processes that make up metabolism in the cell is one of the main challenges of the next century for chemistry.

Nowadays, the most recent advances in laser spectroscopy, microscopy, synthesis, and theory allow probing, describing, and influencing the structure, dynamics, and kinetics of complex solvation phenomena at the molecular level. Ultrashort (ultraviolet, infrared, and terahertz) laser pulses can probe solvent and solute dynamics in real time, scanning tunneling microscopy techniques have been developed which are able to image single solvated molecules on surfaces. Novel stereoselective synthesis strategies are shown to be mediated by the solvent. On the theoretical side, we have witnessed an increase in manageable complexity, which allows an accurate description of solvent–solute interaction beyond the cluster level. Therefore, a molecular-level, bottom-up description of solvation that is able to predict the properties of new solvent systems, also for industrial applications, has come within reach.

The Ruhr-Universität Bochum (RUB) has taken up the challenge of launching solvation science as a new interdisciplinary field at the interface between chemistry, physics, and biology. The goal is to achieve a molecular understanding of the influence of solvation on reactions, biological functions, and processes at liquid–solid interfaces. In 2012, the German Research Foundation (DFG) granted the cluster of excellence "Ruhr Explores Solvation" (RESOLV) 28 million Euros for five years, with RUB as the cluster's host. Fifty research groups from three universities (RUB, Technische Universität Dortmund, and Universität Duisburg-Essen), three Max Planck Institutes (namely Chemical Energy Conversion and Coal Research (both in Mülheim), and Eisenforschung (Iron Research; Düsseldorf)), and the Fraunhofer Institute UMSICHT in Oberhausen are now working together, providing an unprecedented circulation

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of knowledge on the topic of solvation (for more information on RESOLV, see http://www.ruhr-uni-bochum.de/solvation). The sister center CALSOLV (The California Center for Solvation Studies) was founded in 2015 at the College of Chemistry at the University of California, Berkeley. Details are available at http://calsolv.berkeley.edu.

Key to the launch of solvation science is the bringing together and systematic development of a broad array of state-of-the-art synthetic and engineering techniques as well as spectroscopic and theoretical methods. RESOLV is working towards this goal on both a local and global scale. On one hand, a new research building, the Centre of Solvation Science (ZEMOS), is currently being erected on the RUB campus. Funded by the Wissenschaftsrat (WR; German Science Council), it will accommodate about 100 scientists working on solvation science. On the other hand, RESOLV is promoting solvation science knowledge by training young academics and establishing direct collaborations with over 20 top international universities and research institutes, from Yale University to the Weizmann Institute of Science.

Since its launch, RESOLV has already sucessfully pushed back the scientific frontier: Understanding which factors influence a chemical reaction is of key importance for its optimization in both laboratory and industry. Solvation does not only change the properties of reactants and products, but also affects transition states by influencing the thermodynamics, the kinetics, and the product selectivity in liquid-phase reactions. A few solvent molecules are sufficient to change the electronic structure of a molecule and its reactivity completely: A single water or methanol molecule is sufficient to change a highly reactive triplet carbene into a singlet carbene. By using vibrational circular dichroism (VCD), the molecular mechanism of how a chiral anion enforces a chiral conformation onto a catalytically relevant achiral cation could be captured.

Water is the solvent in which life developed. Water may hold the key to the way proteins interact, fold, and misfold in "amyloidic" diseases such as Parkinson's and Alzheimer's. Biomolecular recognition is controlled by a delicate interplay between hydrophobic and hydrophilic interactions.

Within the second research area "solvation and biomolecular function", a new molecular sensor was introduced that allows the influence of the intracellular solvent surroundings on the structure and dynamics of biomolecules to be probed in a spatially resolved way, even within a living cell. The solvent water has been shown to play a crucial role in molecular recognition: When an enzyme interacts with this solvent, a gradient of hydrogen-bond dynamics with more and more retarded water molecules towards the active site, the so-called "hydration funnel", is formed. This slowing down of water dynamics is found to be crucial in order to minimize the entropic cost for binding of the substrate at the catalytic site.

The third research area of RESOLV focuses on the understanding of solvation, charge transfer, and (electro-)chemical reactions at interfaces. Over the last few decades, surface science has triggered an impressive boost in the molecular understanding of catalytic processes on surfaces. However, this has mainly been restricted to reactions at the gas–solid interface, while little is known about how reactants become desolvated, intermediates stabilized, and products resolvated along catalytic cycles at liquid–solid interfaces. White-light interferometry was used as a unique real-time tool to visualize dynamic processes at electrochemically active metal interfaces with Ångström resolution. This study underlined the importance of the interfacial solvent for electrochemical reactions at the metal interfaces. Moreover, thin water layers confined between surfaces are known for their surprising properties. Indeed, it turns out that excess protons hosted in nanosized water films intercalated in a layered mineral still undergo efficient Grotthuss diffusion akin to bulk water, as ab initio computer simulations have unveiled. Current research suggests that nanoconfinement strongly impacts not only the energetic barriers of chemical reactions, but also the reaction mechanisms.

Transcending the traditional view, solvents are now increasingly recognized as playing an active role in their own right in various processes, ranging from solvent-mediated to solvent-controlled, and even to solvent-steered ones. These developments are the first steps on the long path towards application, for example, the development of the next generation of batteries. To transfer the new concepts and the new discoveries into real-life applications, large collaborative interdisciplinary projects like RESOLV are the way forward. Solvation science will provide the unifying framework for understanding and predicting solvent processes and this knowledge will be then transferred directly into applications. Thanks to the technologies now at our disposal, it is finally possible to give solvents the importance that ancient philosophers once granted to them. In the light of such exciting prospects, solvation science is here to stay.

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